Numerical methods for FEL oriented - plasma accelerators

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Outline

- **Plasma simulations for plasma-based FEL experiments**
  - Motivation, Tradeoff data /simulation and development time
- **Basics of PIC simulations**
  - Basic PIC loop, Additional features
- **How can I speed up my simulations?**
  - QSA, Boosted frame
  - Hybrid codes, Azimuthal decomposition

Role of Plasma simulation in FEL experiments

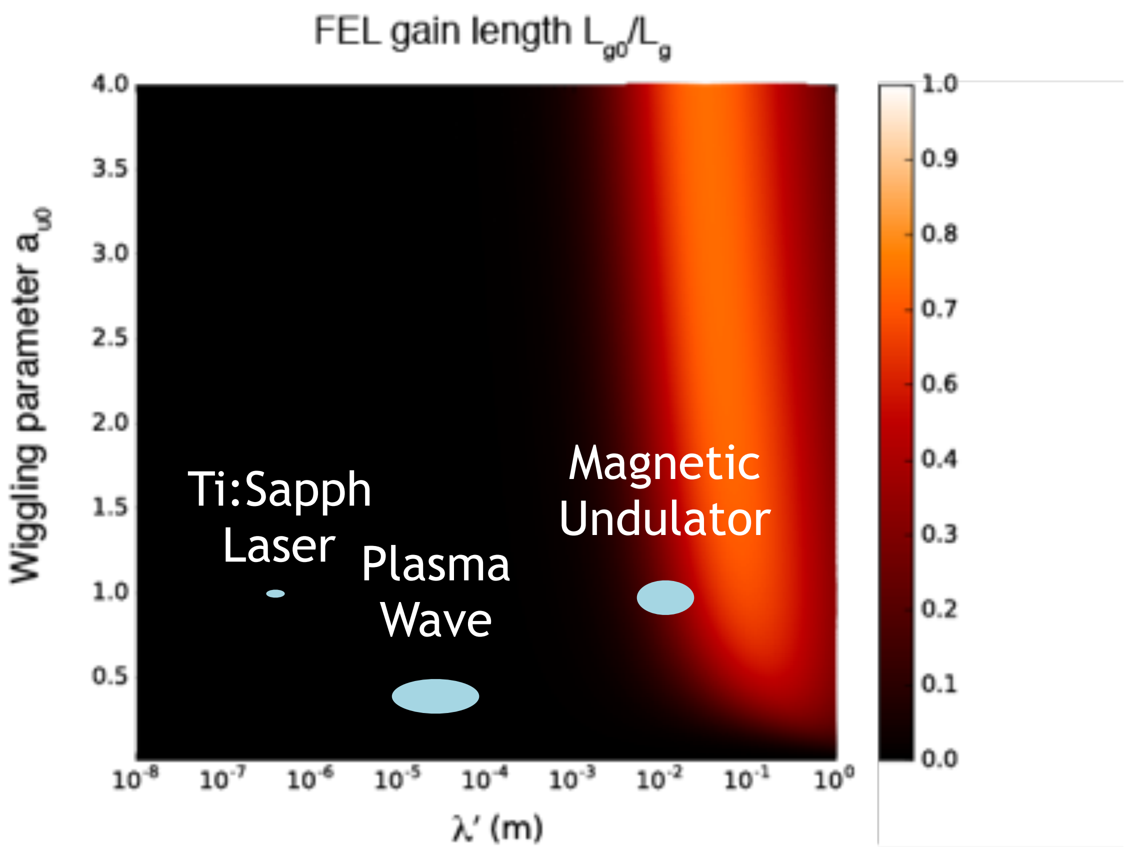
- Design new experiments / Improve existing designs
- Investigating underlying physical mechanisms
- Understanding experimental results

Example: Simulate plasma accelerated beams to design plasma - based FEL experiments

My simulations say that in idealised cases I can produce a LWFA electron beam with:

I = 30 kA, γ = 400, σ_γ/γ = 1%, ε_x = 0.5 mm-mrad, σ_x =100 μm

Xie's formulas: can the beam be used for FEL? Which kind of undulator suits best?



M. Xie, Nucl. Instr. and Meth. A 445 (2000)

Physical realism: nothing is given for free

Speed in simulations and code development

1D codes

2D codes

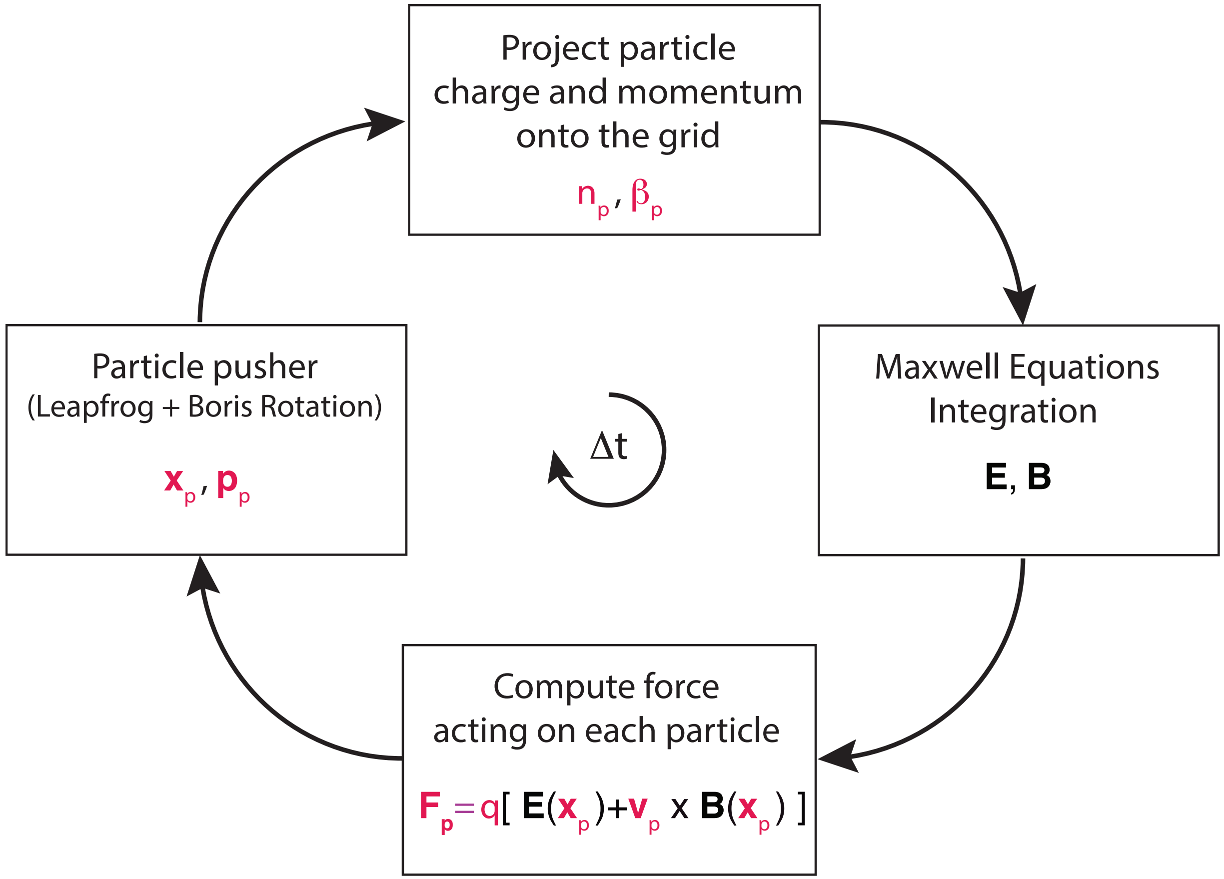
3D codes

Physics included, Amount of available output

Basic Particle in Cell (PIC) Loop

Plasma = **computational macroparticles** moved by **E. M. fields** they induce on a grid

C. K. Birdsall, A. B. Langdon, Plasma Physics Via Computer Simulation



download a Python 1D PIC code by A. Marocchino: http://gaps.ing2.uniroma1.it/alberto/alberto/PIC.html

PIC codes: additional features

- Moving window (mandatory for long propagation lengths)
- Parallelisation (mandatory for 2D-3D simulations)
- Flexible and quick output analysis
- Collisions
- Ionisation (Field Ionisation / Collision Ionisation)
- Reaction Force
- QED effects (e.g. pair production)

More Physics, more data

=

More time to run simulations and to develop codes

Quasi-Static Approximation (QSA)

Assumption: driver evolution much slower than background plasma evolution, i.e. driver can be considered frozen while plasma electrons pass it

(Laser diffraction time or betatron period ω_β^{-1} >> Plasma period ω_p^{-1})

Introducing new variables:

$\tau = t,$

$\zeta = z - ct$ (Comoving variable)

→ QSA: neglect τ derivatives with respect to ζ derivatives for background plasma

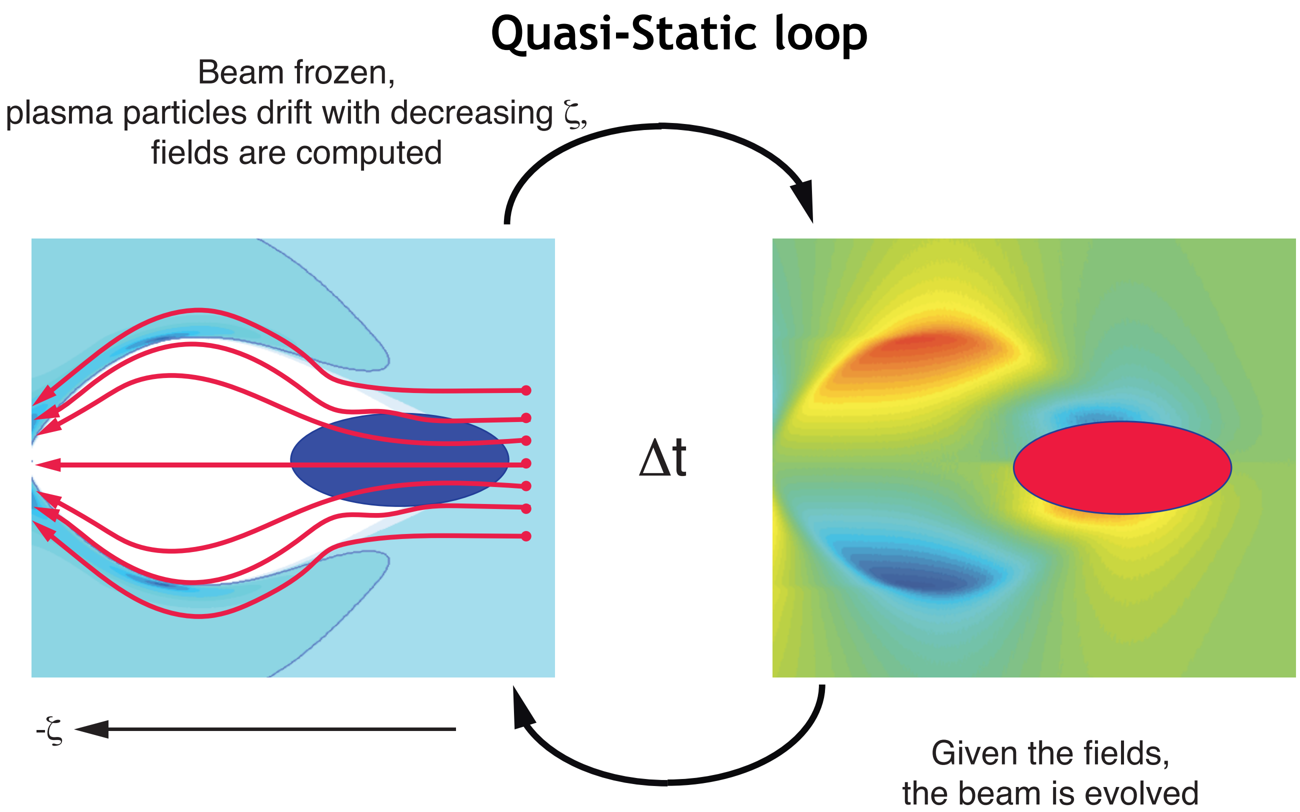
In QSA the τ dependance in the fields and plasma quantities disappears

Plasma quantities at each iteration depend only on the distance from the driver ζ

Transversely, the fields (or potentials) equations are no more local

Quasi-Static Loop(QSA)

- Plasma particles are initialised ahead of the driver (ζ>0) and then evolved drifting along the frozen driver, integrating along ζ
- The fields by driver and background are computed
- The driver is pushed by the fields



Quasi-Static Approximation (QSA): Performances

Speed-up

$\sim(2\gamma_{driver})^{1/2}$ for PWFA

$\sim(\lambda_p/\lambda_0)^2$ for LWFA

Disadvantages

- Radiation is not included
- Injection, trapping, wave breaking are not reproduced
- Sharp longitudinal variations in initial plasma density violate QSA assumptions (τ derivatives are no more negligible)

Examples of codes with QSA (not exhaustive list):

- **WAKE**

P. Mora and T. M. Antonsen, *Phys. Rev.* E **53** R2068 (1996)
P. Mora and T. M. Antonsen, *Phys. Plasmas* **4** 217 (1997)

- **LCODE (electron PWFA, QSA, full PIC/hybrid modes available)**

K. V. Lotov, Physics of Plasmas 5, 785 (1998); doi: 10.1063/1.872765, http://www.inp.nsk.su/~lotov/lcode/

- **QuickPIC (time explicit, PWFA and LWFA)**

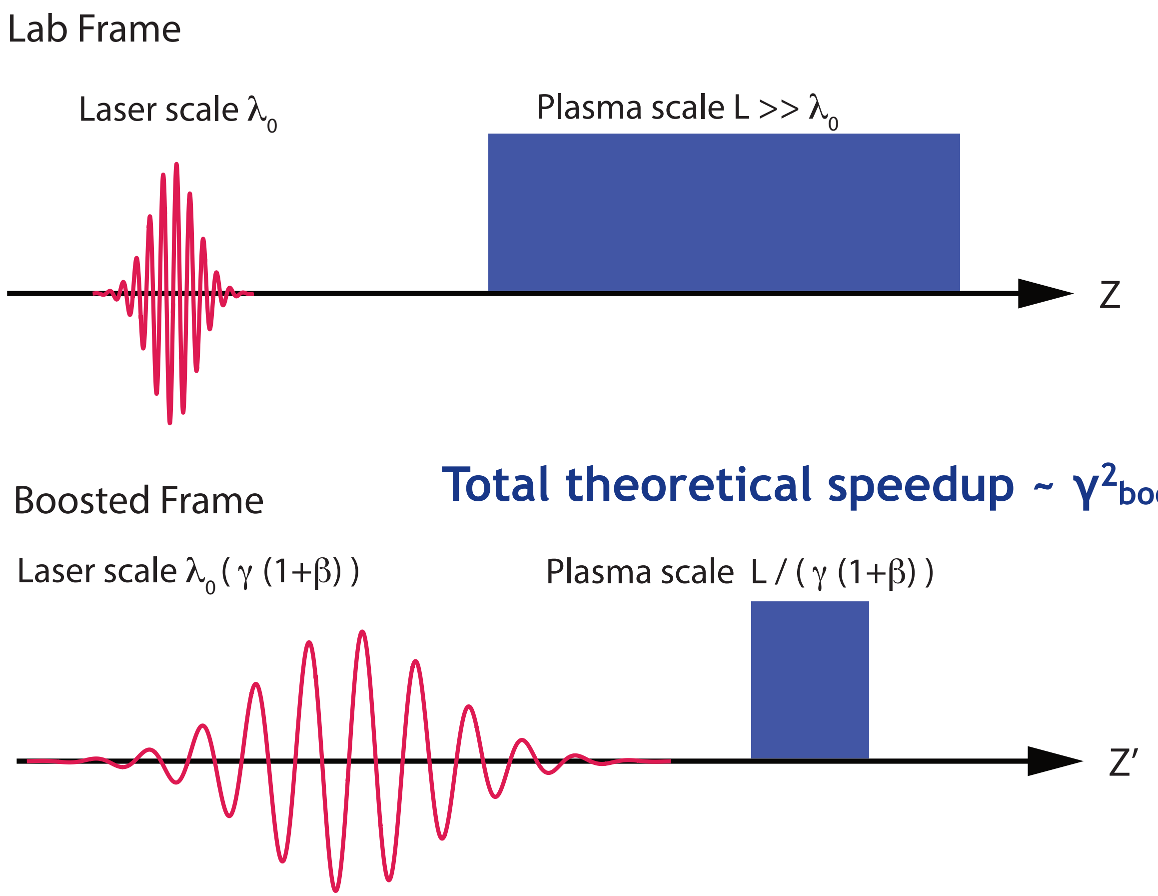
C. Huang et al, J .Comput.Phys. **217**658, (2006)
B. Feng et al, J.Comput. Phys. **228**5340 (2009)
W. An et al, J. Comput. Phys. **250** 165 (2013)

Lorentz Boosted Frame simulations

In a boosted frame moving with relativistic factor γ_{boost}

- the driver is stretched by γ_{boost} (coarser grid cell size possible)
- the plasma channel is compressed by factor γ_{boost} (smaller distance to travel)

J.-L. Vay, *Phys. Rev. Lett.* 98 (2007) 130405. http://dx.doi.org/10.1103/PhysRevLett.98.130405

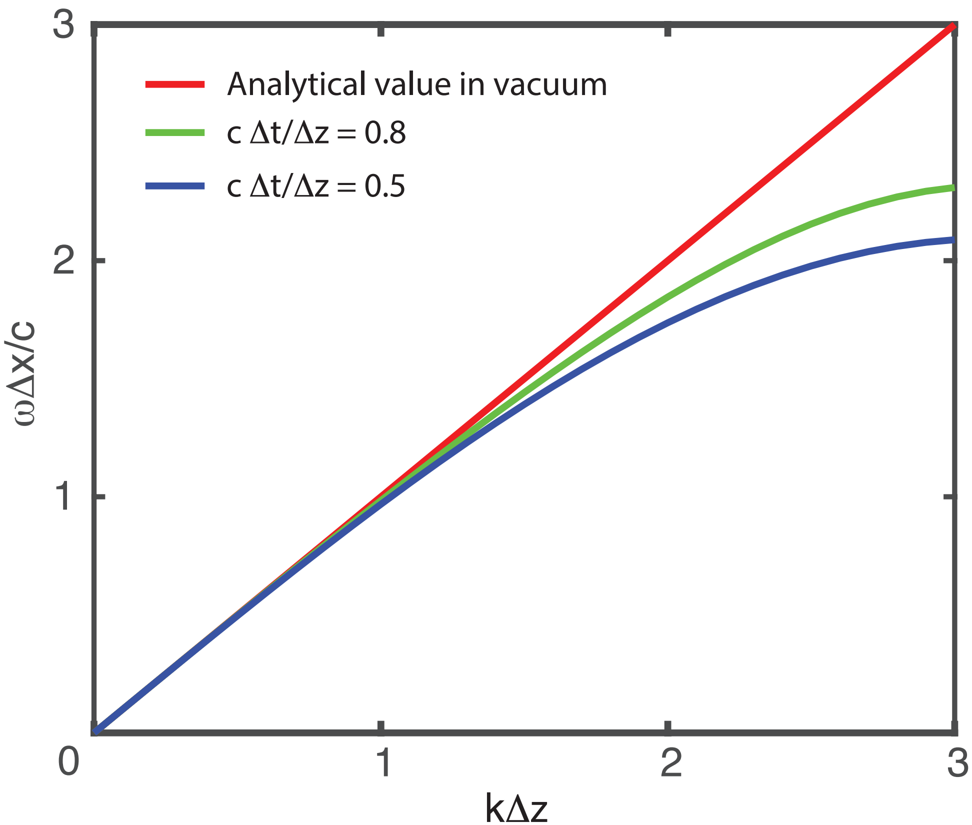


Total theoretical speedup ~ γ^2_{boost}

Boosted frame: numerical Cherenkov instability

Numerical dispersion in standard PIC codes (FDTD scheme) slows down radiation, radiation deflects particles, generated current induces more radiation

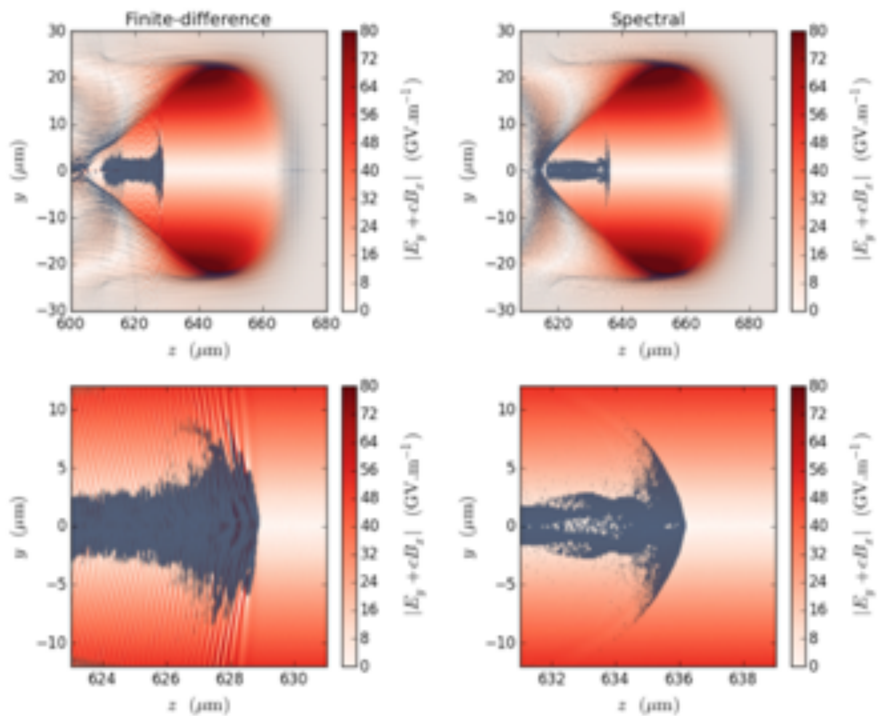
B. B. Godfrey, "Numerical Cherenkov instabilities in electromagnetic particle codes", *J. Comput. Phys.* **15** (1974)

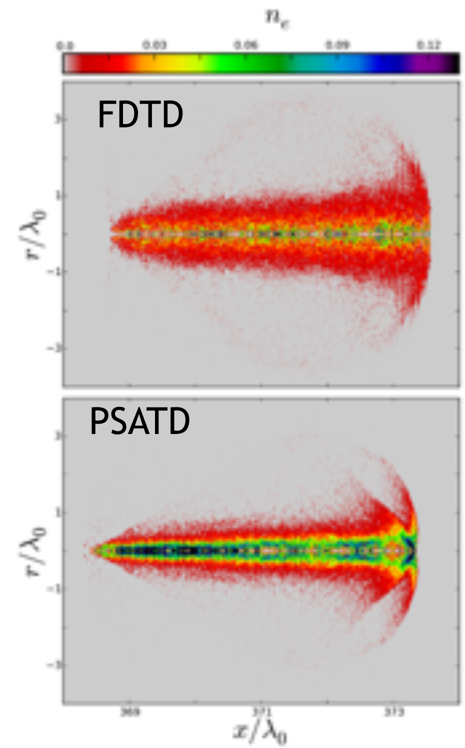


In boosted frame codes there are many particles moving at speed near c, thus numerical Cherenkov instability grows more quickly

Numerical dispersion - free codes

Dispersion - free algorithms (e.g. Pseudo-Spectral Analytical Time Domain) mitigate numerical Cherenkov instability





R. Lehe, M. Kirchen, I. A. Andriyash, B. Godfrey, J.-L. Vay, "A spectral, quasi-cylindrical and dispersion-free Particle-In-Cell algorithm", *Computer Physics Communications 203 (2016) 66-82*.

I. A. Andriyash, R. Lehe, A. Lifschitz, "Laser-plasma interactions with a Fourier-Bessel particle-in-cell method", Phys. Plasmas **23**, 033110 (2016)

Hybrid kinetic - fluid codes

Most cumbersome PIC routines:
- Particle Push,
- Particle Charge deposition, Computation of Forces on Particles from grid

Hybrid code = Beam Particles / Laser + Fluid Plasma Electron Background

Background advance reduces to solve fluid equations on grid (dramatic speedup)
Disadvantages: **kinetic effects, highly nonlinear regimes are not included**

Examples of hybrid codes:

- **LCODE (electron PWFA, QSA, includes also full PIC mode)**

K. V. Lotov, Physics of Plasmas 5, 785 (1998); doi: 10.1063/1.872765, http://www.inp.nsk.su/~lotov/lcode/

- **INF&RNO (for LWFA, with/without QSA, includes also full PIC mode)**

C. Benedetti et al, Proceedings of ICAP2012, ISBN 978-3-95450-116-8

- **H-VLPL3D (time explicit, for proton PWFA)**

T. Tückmantel, A. Pukhov, Journal of Computational Physics 269 (2014) 168–180

- **Architect (time explicit, electron PWFA)**

A.Marocchino, F. Massimo et al, Nucl. Instr. and Meth. A (2016) http://dx.doi.org/10.1016/j.nima.2016.03.005,
A.Marocchino, F. Massimo, http://dx.doi.org/10.5281/zenodo.49572, (2016).

Example: Architect Model

Beam Particles + Fluid Plasma Electron Background

$$d_t \mathbf{p}_{\text{particle}} = q(\mathbf{E} + c\boldsymbol{\beta}_{\text{particle}} \times \mathbf{B})$$

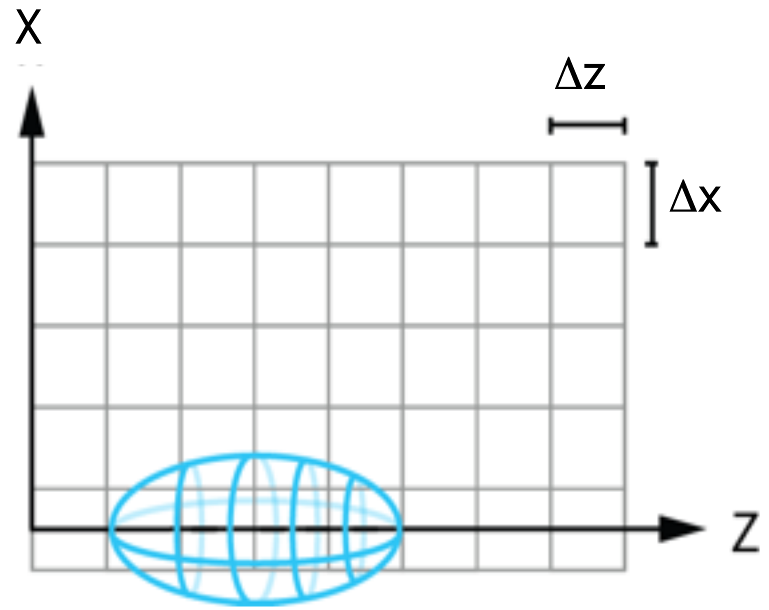
$$d_t \mathbf{x}_{\text{particle}} = \boldsymbol{\beta}_{\text{particle}} c$$

$$\partial_t n_e = -\nabla \cdot (\boldsymbol{\beta}_e c n_e)$$

$$\partial_t \mathbf{p}_e = -\nabla \cdot (\mathbf{p}_e \otimes \boldsymbol{\beta}_e c) + q(\mathbf{E} + c\boldsymbol{\beta}_e \times \mathbf{B})$$

$$\partial_t \mathbf{B} = -\nabla \times \mathbf{E}$$

$$\partial_t \mathbf{E} = c^2 \nabla \times \mathbf{B} - q\mu_0 c^3 (n_e \boldsymbol{\beta}_e + n_b \boldsymbol{\beta}_b)$$

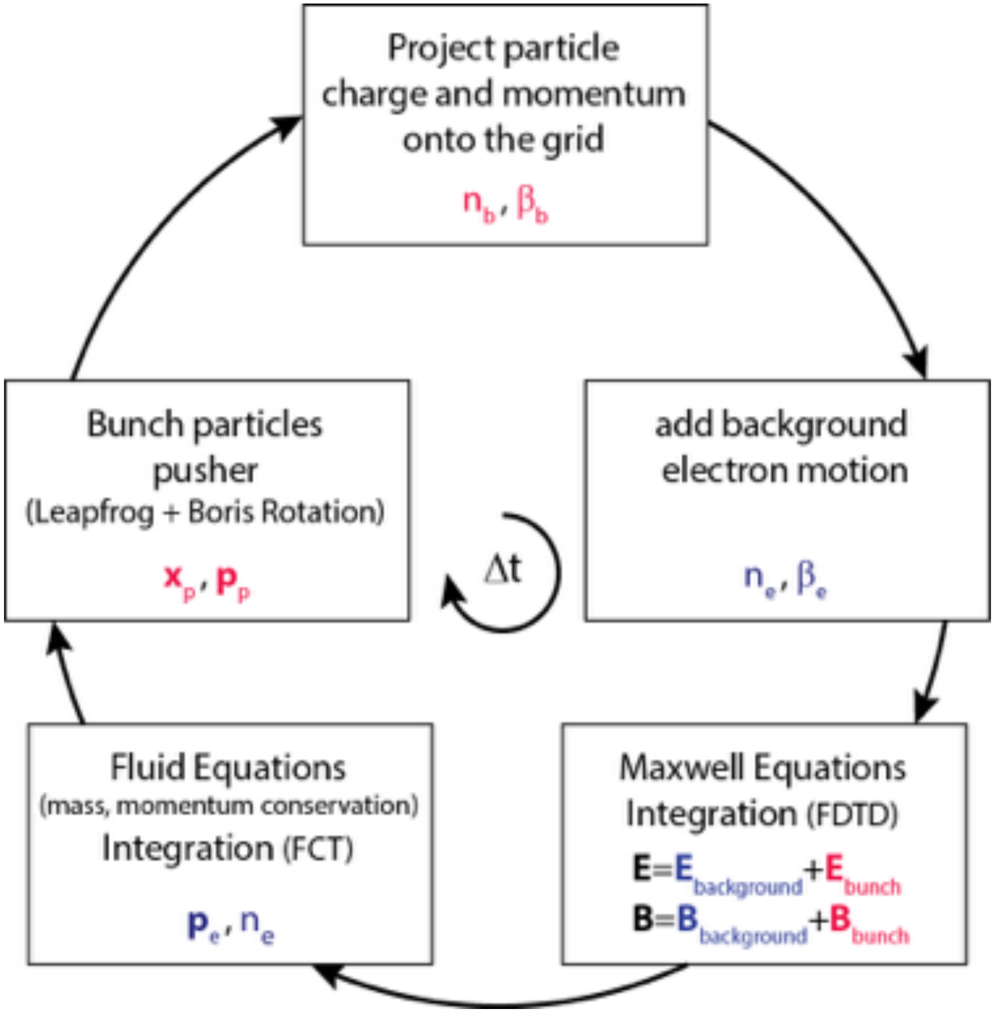


- Beam particles move in 3D-3V space
- EM fields and fluid integration in moving window, no quasi-static approximation
- **cylindrical symmetry** assumed for fluid and electromagnetic fields (Z, X, X>0)
- Only X>0 domain is considered in the fluid and electromagnetic field equations
- **No need for parallelization** for typical SPARC_LAB simulations

Architect: first release, A. Marocchino, F. Massimo, http://dx.doi.org/10.5281/zenodo.49572 (2016).

Example: Architect Loop

Beam Particles + Fluid Plasma Electron Background



Architect: Comparison against 3D PIC code ALaDyn

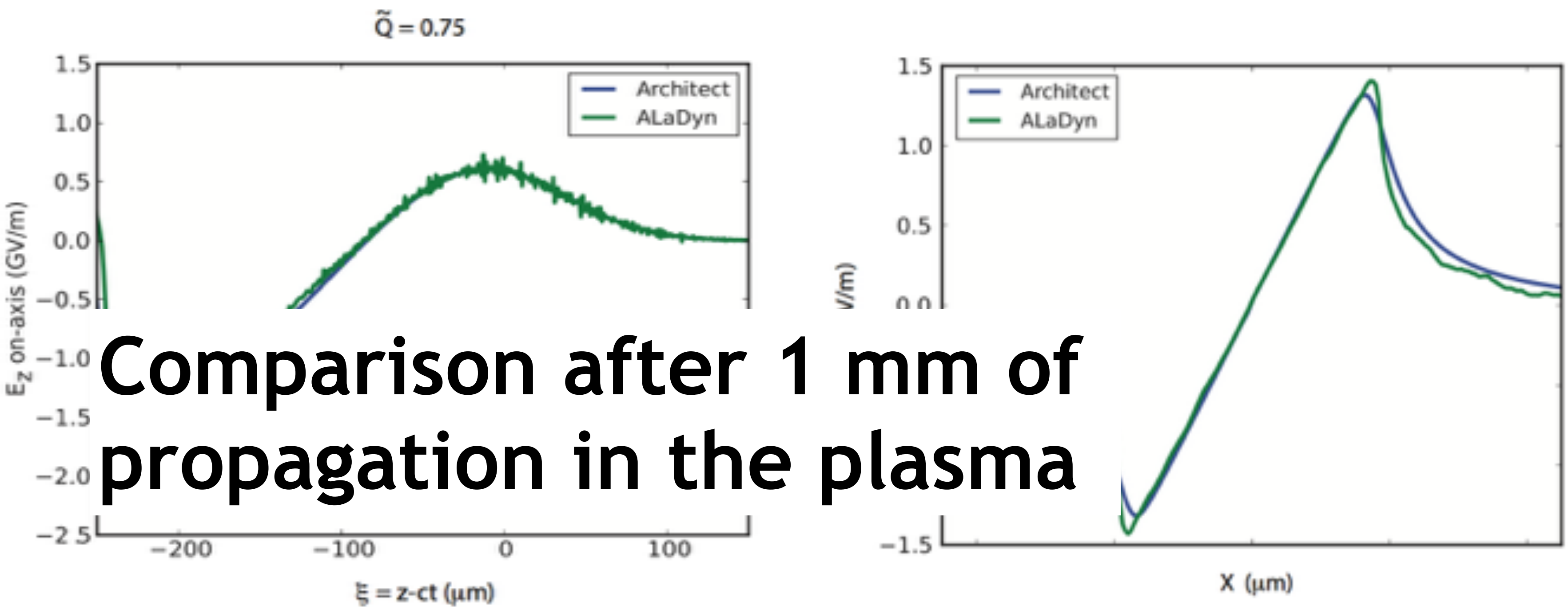
- Q = 180 pC
- σ_x = 9 μm, σ_z = 50 μm
- E_0 = 100 MeV
- ε_x = 1 mm-mrad
- $\Delta\gamma/\gamma$ = 0.1%
- n_0 = 10^{16} cm^{-3}

3D ALaDyn simulation

- **4 kh-cores run time**
- 106 Mcells
- 850 Mparticles
- Δt = 0.23 fs
- Δx = 0.4 μm
- Δz = 1 μm

2D Architect simulation

- **1 hour run time (1 cpu)**
- 250 cells
- 15 kparticles
- Δt = 0.2 fs
- Δr = 0.4 μm
- Δz = 1 μm



Comparison after 1 mm of propagation in the plasma

ALaDyn v1.0.0-beta, S. Sinigardi, A. Marocchino, P. Londrillo, A. Sgattoni, http://dx.doi.org/10.5281/ zenodo.49553 (2016).

Architect: first release, A. Marocchino, F. Massimo, http://dx.doi.org/10.5281/zenodo.49572 (2016).

Azimuthal Fourier decomposition

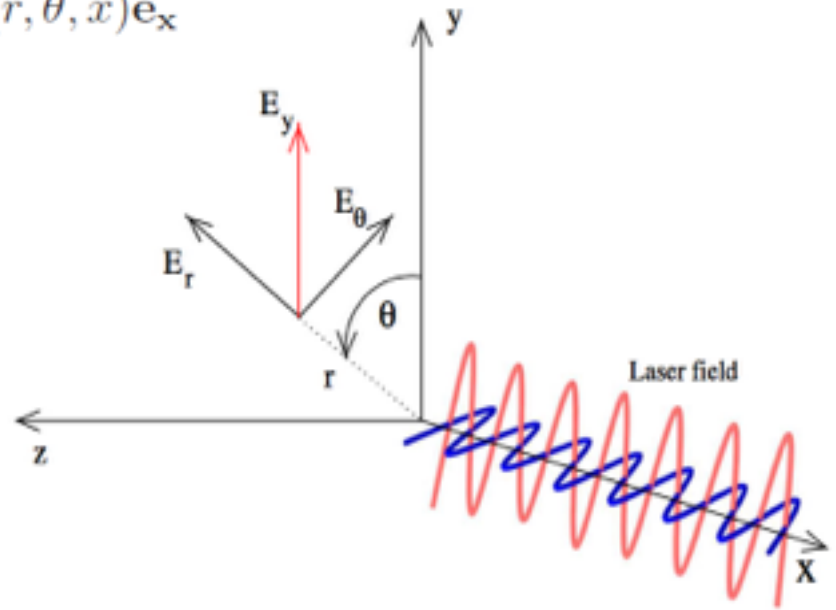
- Cylindrical coordinates are used for the fields:

$$\mathbf{E}(r,\theta,x) = E_r(r,\theta,x)\mathbf{e_r} + E_\theta(r,\theta,x)\mathbf{e}_\theta + E_x(r,\theta,x)\mathbf{e_x}$$

- Fourier decomposition is used in the azimuthal coordinate

$$F(r,\theta,x) = \sum_{m=-\infty}^{+\infty} \hat{F}^m(r,x)e^{-im\theta}$$

$$\hat{F}^m(r,x) = \frac{1}{2\pi}\int_0^{2\pi} F(r,\theta,x)e^{im\theta}d\theta$$



- Often for LWFA only few azimuthal modes are needed

- Neglecting all but the first N modes, cost is approximately equal to N 2D simulations

Example:

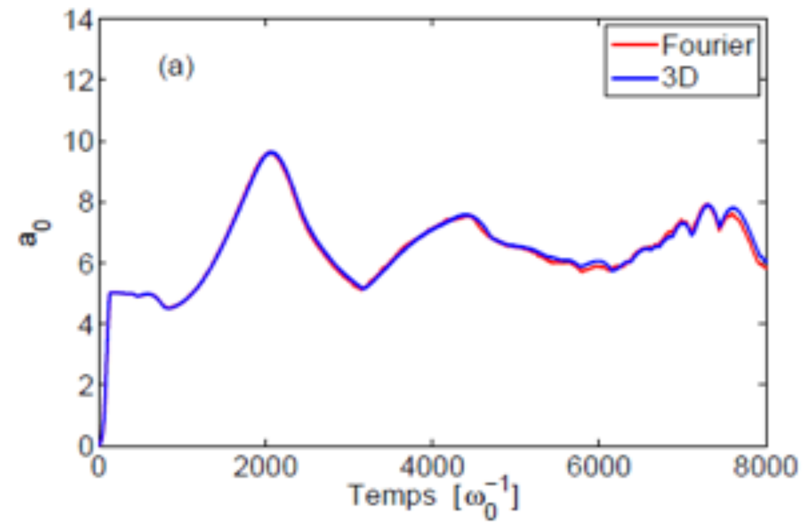
CALDER-CIRC

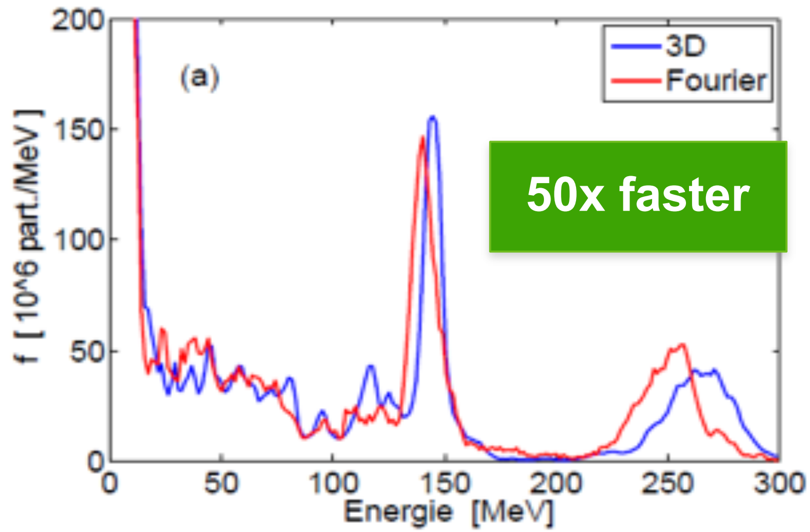
X. Davoine et al. “New Algorithms for Cylindrical PIC code” (1st EAAC - 2013)
A. Lifschitz et al, Journal of Computational Physics 228 (2009)

Azimuthal Fourier decomposition: comparisons of CALDER-CIRC with full 3D code

Laser and plasma parameters

- λ_0 = 0.8 µm
- τ_0 = 30 fs
- w_0 = 9 µm
- a_0 = 5
- ne = 0.007 nc





50x faster

Images from X. Davoine et al. “New Algorithms for Cylindrical PIC code” (1st EAAC - 2013)

A. Lifschitz et al, Journal of Computational Physics 228 (2009)

Summary

- PIC codes are essential tools to investigate various regimes of plasma acceleration, including plasma sections of plasma-based FEL
- Huge amounts of data in PIC codes slow down the simulation
- Various “tricks” and reduced models can be used to speed up simulations, as QSA, Boosted Frame, Azimuthal decomposition, Hybrid kinetic-fluid codes
- Advantages of the various solutions must be weighted with the physics they lose
- Joint use of different models can address speed/accuracy demands

Acknowledgements

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